CLAIMS

What is claimed as new and desired to be protected by Letters Patent of the United States is:

1. A system for improved modeling of a biological system that comprises a plurality of chemical reactions, the system comprising:

a modeling component comprising a graphical user interface for accepting user commands and input to construct a model of the biological system;

a simulation engine accepting as input said constructed model of the biological system and generating as output dynamic behavior of the biological system; and

an analysis environment in communication with said simulation engine, said analysis environment displaying dynamic behavior of the biological system.

2. The system of claim 1 wherein the modeling component allows construction of a block diagram model of the biological system. .

3. The system of claim 2 wherein the modeling component further includes at least one block identifying a set of related chemical reactions.

4. The system of claim 1 wherein the modeling component includes a tool palette for aiding construction of the model of the biological system.

5. The system of claim 1 wherein said simulation engine generates the dynamic behavior of the biological system using a stochastic computational model.

6. The system of claim 1 wherein said simulation engine generates the dynamic behavior of the biological system using a discrete time-based computational model.

7. The system of claim 1 wherein said simulation engine generates the dynamic behavior of the biological system using a continuous time-based computational model.

8. An improved method for modeling a biological process comprising a plurality of chemical reactions, the method comprising the steps of:

(a)   providing a graphical user interface for accepting user commands and data;

(b)   receiving, via the provided user interface, user commands and data;

(c)   constructing, using the received user commands and data, a model of the biological process;

(d)   generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process; and

(e)   displaying the dynamic behavior of the biological process on a display device.

9. The method of claim 8 wherein step (c) comprises constructing a block diagram model of the biological process.

10. The method of claim 9 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

11. The method of claim 8 wherein step (d) comprises generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a stochastic computational model.

12. The method of claim 8 wherein step (d) comprises generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a discrete time-based computational model.

13. The method of claim 8 wherein step (d) comprises generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a continuous time-based computational model.

14. An article of manufacture having embodied thereon computer-readable program means for improved modeling of a biological process comprising a plurality of chemical reactions, the article of manufacture comprising:

computer-readable program means for providing a graphical user interface for accepting user commands and data;

computer-readable program means for receiving, via the provided user interface, user commands and data;

computer-readable program means for constructing, using the received user commands and data, a model of the biological process;

computer-readable program means for generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process; and

computer-readable program means for displaying the dynamic behavior of the biological process.

15. The article of manufacture of claim 14 wherein said computer-readable program means for constructing a model of the biological process comprises computer-readable program means for constructing a block diagram model of a biological process.

16. The article of manufacture of claim 15 wherein said computer-readable program means for constructing a block diagram model of the biological process includes computer-readable program means for constructing at least one block identifying a set of related chemical reactions.

17. The article of manufacture of claim 14 wherein computer-readable program means for generating dynamic behavior of the modeled biological process comprises computer-readable program means for generating dynamic behavior of the modeled biological process using a stochastic computational model.

18. The article of manufacture of claim 14 wherein computer-readable program means for generating dynamic behavior of the modeled biological process comprises computer-readable program means for generating dynamic behavior of the modeled biological process using an event-based computational model.

19. The article of manufacture of claim 14 wherein computer-readable program means for generating dynamic behavior of the modeled biological process comprises computer-readable program means for generating dynamic behavior of the modeled biological process using a continuous time-based computational model.

20. A system for improved modeling of a chemical reaction comprising:

a modeling environment accepting user commands and input for constructing a model of a chemical reaction;

a simulation engine accepting as input said constructed model of the chemical reaction and generating as output an expected result; and

an analysis environment in communication with said simulation engine, said analysis environment displaying the expected result.

21. The system of claim 20 wherein the modeling environment allows construction of a block diagram model of a chemical reaction.

22. The system of claim 21 wherein the modeling environment further includes at least one block identifying a set of related chemical reactions.

23. The system of claim 20 wherein said simulation engine generates an expected result using a stochastic computational model.

24. The system of claim 20 wherein said simulation engine generates an expected result using a discrete time-based computational model.

25. The system of claim 20 wherein said simulation engine generates an expected result using a continuous time-based computational model.

26. A method for integrated modeling, simulation and analysis of chemical reactions, the method comprising the steps of:

(a) providing a graphical user interface for accepting user commands and data;

(b) receiving, via the provided user interface, user commands and data;

(c) constructing, using the received user commands and data, a model of a chemical reaction;

(d) generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction; and

(e) displaying the expected result.

27. The method of claim 26 wherein step (c) comprises constructing a block diagram model of a chemical reaction.

28. The method of claim 27 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

29. The method of claim 26 wherein step (d) comprises generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a stochastic computational model.

30. The method of claim 26 wherein step (d) comprises generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a discrete time-based computational model.

31. The method of claim 26 wherein step (d) comprises generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a continuous time-based computational model.

32. An article of manufacture having embodied thereon computer-readable program means for integrated modeling, simulation and analysis of chemical reactions, the article of manufacture comprising:

computer-readable program means for providing a graphical user interface for accepting user commands and data;

computer-readable program means for receiving, via the provided user interface, user commands and data;

computer-readable program means for constructing, using the received user commands and data, a model of a chemical reaction;

computer-readable program means for generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction; and

computer-readable program means for displaying the expected result.

33. The article of manufacture of claim 32 wherein said computer-readable program means for constructing a model of the chemical reaction comprises computer-readable program means for constructing a block diagram model of a chemical reaction.

34. The article of manufacture of claim 33 wherein said computer-readable program means for constructing a block diagram model of the chemical reaction includes computer-readable program means for constructing at least one block identifying a set of related chemical reactions.

35. The article of manufacture of claim 32 wherein computer-readable program means for generating an expected result of the modeled chemical reaction comprises computer-readable program means for generating an expected result of the modeled chemical reaction using a stochastic computational model.

36. The article of manufacture of claim 32 wherein computer-readable program means for generating an expected result of the modeled chemical reaction comprises computer-readable program means for generating an expected result of the modeled chemical reaction using an event-based computational model.